Diffraction in Time: An Exactly Solvable Model

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In the recent years, mater-wave interferometry has attracted growing attention due to its unique suitability for high-precision measurements and study of fundamental aspects of quantum theory. Diffraction and interference of matter waves can be observed not only at a spatial aperture (such as a screen edge, slit, or grating), but also at a time-domain aperture (such as an absorbing barrier, or "shutter", that is being periodically switched on and off). The wave phenomenon of the latter type is commonly referred to as "diffraction in time". Here, we introduce a versatile, exactly solvable model of diffraction in time. It describes time-evolution of an arbitrary initial quantum state in the presence of a time-dependent absorbing barrier, governed by an arbitrary aperture function. Our results enable a quantitative description of diffraction and interference patterns in a large variety of setups, and may be used to devise new diffraction and interference experiments with atoms and molecules.

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The wave nature of matter is both captivating and perplexing, and its exploration has been at the center of experimental and theoretical research since early days of quantum mechanics. To date, diffraction and interference experiments have been successfully performed with particles ranging from elementary particles and simple atoms to complex molecular clusters [1, 2]. Most spectacularly, wave-like behavior has been convincingly demonstrated even for such large organic compounds as $C_{60}[C_{12}F_{25}]_{10}$ and $C_{168}H_{94}F_{152}O_8N_4S_4$, each comprising 430 atoms [3].

In optics, diffraction is typically portrayed as deflection of light incident upon an obstacle with sharp boundaries, that can not be accounted for by reflection or refraction. Interestingly, quantum mechanics allows for an additional, intrinsically time-dependent manifestation of the phenomenon: Owing to the dispersive nature of quantum matter waves, sudden changes in boundary conditions may cause the particle wave function to develop interference fringes akin to those in stationary (optical) diffraction problems. This phenomenon, pioneered in 1952 by Moshinsky [4] and presently referred to as "diffraction in time" (DIT), is at the heart of a vibrant area of experimental and theoretical research concerned with quantum transients (see Ref. [5] for a review).

In the original Moshinsky's setup [4], a monoenergetic beam of non-relativistic quantum particles is incident upon a perfectly absorbing barrier ("shutter"). The shutter is suddenly removed at time $t = t_1$. In other words, the transparency of the barrier $\chi(t)$, called the aperture function, jumps instantaneously from 0 at $t < t_1$ to 1 at $t > t_1$, i.e., $\chi(t) = \Theta(t - t_1)$, with Θ denoting the Heaviside step function. The removal of the shutter renders a quantum wave function with a sharp, discontinuous wave front. The latter disperses in the course of time, smoothing out the initial discontinuity and developing a sequence of interference fringes. As Moshinsky has shown, these fringes bear close mathematical similarity to those in Fresnel diffraction of light at the edge of a straight, semi-infinite screen. Moshinsky's paradigmatic triggered considerable interest to DIT in experimental research with ultra-cold neutrons and atoms, and Bose-Einstein condensates [1, 2, 5].

On the theoretical side, a number of interesting extensions and variations of Moshinsky's shutter problem have been addressed. Moshinsky himself extended his original result to the case of a "time slit", in which the shutter stays open only during a time interval $t_1 < t < t_2$, as described by the aperture function $\chi(t) = \Theta(t-t_1)\Theta(t_2-t)$ [6]. Scheitler and Kleber found an exact analytical solution of a related problem, in which the role of a smoothly opening shutter was played by a time-dependent δ-potential barrier $V(x,t) \sim t^{-1}\delta(x)$, with x denoting the spatial coordinate [7, 8]. Various physical problems, requiring generalization of the original Moshinsky's setup to describe DIT caused by an arbitrary aperture function, $\chi(t)$, have been addressed in Refs. [9–14]. The analytical methods adopted in all these studies rely on treating the shutter as an effective "source" boundary of a semi-infinite coordinate space (transmission region). The main advantage of this approach is that the transmitted wave can be readily expressed in terms of $\chi(t)$ and a time-dependent source boundary condition. A significant difficulty with this approach however is that, in general, there is no unique well-defined recipe for finding the source function that would accurately mimic a given incident wave packet (although, in some cases, efficient approximations and exact bounds are known [12]).

In this paper, we introduce a self-consistent *exactly solvable* model of DIT, free of arbitrary parameters. The model aims to describe dynamics of an *arbitrary quan-*

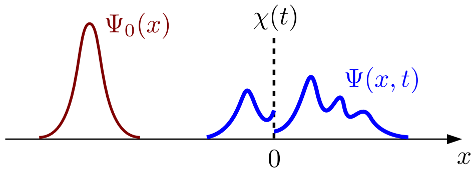

FIG. 1: Illustration of time-evolution of a quantum state in the presence of a time-dependent absorbing shutter.

tum state in the presence of an absorbing time-dependent shutter characterized by an *arbitrary aperture function* $\chi(t)$, see Fig. 1. It serves as a versatile generalization of the original Moshinsky's problem and reduces to the latter in the particular case $\chi(t) = \Theta(t - t_1)$.

The central quantity analyzed in this paper is a propagator $K(x, x'; t)$ that relates the particle wave function $\Psi(x, t)$ at time $t > 0$ to an initial quantum state $\Psi_0(x)$ at $t = 0$ through [15]

$$\Psi(x,t) = \int_{-\infty}^{+\infty} \mathrm{d}x'\, K(x, x'; t)\Psi_0(x')\,. \tag{1}$$

The propagator satisfies the time-dependent Schrödinger equation (TDSE) on both sides of the absorbing shutter, positioned at $x = 0$, i.e.,

$$\left(i\partial_t + \frac{\hbar}{2m}\partial_x^2\right) K(x, x'; t) = 0 \quad \text{for} \quad x, x' \neq 0\,. \tag{2}$$

Here, m denotes the mass of the particle. The propagator is subject to the initial condition

$$K(x, x'; 0^+) = \delta(x - x')\,, \tag{3}$$

and is required to vanish as $x \to \pm\infty$ at negative imaginary times, i.e., at $t = -i|t|$.

Our treatment of absorption is based on a time domain rendition of an approach originally introduced by Kottler. The approach applies to diffraction of stationary fields governed by the Poisson's equation at spatial apertures in otherwise perfectly absorbing ("black") screens [16, 17]. According to this approach, a wave originating on one side of a black screen is subject to a discontinuous jump at every point of the screen, except for points inside possible openings (holes, slits, etc.). More concretely, the difference of the wave amplitude on the source side of the screen and that on the opposite side equals the amplitude of the corresponding free-space wave, i.e., the amplitude the wave would have if no screen were present. A similar discontinuity condition is imposed on the normal derivative of the field. Both the field and its normal derivative are postulated continuous across the openings. As Kottler has shown, an exact solution of the Poisson's equation, subject to the above well-defined, though unusual, discontinuous boundary conditions, is identical to the wave field predicted by Kirchhoff's diffraction theory.

In our model, we consider a time-dependent generalization of the Kottler's discontinuity condition at the shutter. Thus, we require the propagator to satisfy

$$K(x, x'; t)\big|_{x=0^-}^{x=0^+} = \mathrm{sgn}(x')\big[1 - \chi(t)\big] K_0(x - x', t)\big|_{x=0} \tag{4}$$

and

$$\partial_x K(x, x'; t)\big|_{x=0^-}^{x=0^+} = \mathrm{sgn}(x')\big[1 - \chi(t)\big]\partial_x K_0(x - x', t)\big|_{x=0}\,. \tag{5}$$

Here, $\chi(t)$ denotes the aperture function, ranging between 0 (shutter closed) and 1 (shutter open),

$$K_0(z, t) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(i\frac{m}{2\hbar t}z^2\right) \tag{6}$$

is the free-particle propagator, and $\mathrm{sgn}(x') = x'/|x'|$ stands for the sign function. The latter identifies whether the source is located to the left or right of the shutter.

Equations (2–5) completely specify dynamics of a quantum particle in the presence of a time-dependent absorbing barrier. In fact, as will be shown below, this quantum-mechanical problem admits an exact analytic solution valid for an arbitrary piecewise differentiable function $\chi(t)$. The solution is given by

$$K(x, x'; t) = \Xi(x, x')K_0(x - x', t) + K_1(x, x'; t) \tag{7}$$

with

$$K_1(x, x'; t) = \int_0^t \mathrm{d}\tau\, u\, K_0(x, t - \tau)\chi(\tau)K_0(-x', \tau) \tag{8}$$

and

$$u(x, x'; t, \tau) = -\frac{\mathrm{sgn}(x')}{2}\left(\frac{x}{t - \tau} - \frac{x'}{\tau}\right)\,. \tag{9}$$

Here, $\Xi(x, x') = [1 + \mathrm{sgn}(x)\mathrm{sgn}(x')]/2$, i.e., Ξ equals 1 if x and x' lie on the same side of the barrier, and 0 otherwise.

For what follows below, it is useful to rewrite the propagator, given by Eqs. (7–9), in an alternative form. Evaluating the integral in Eq. (8) by parts, we obtain

$$K(x, x'; t) = \Xi(x, x')\big[1 - \chi(t)\big]K_0(x - x', t) + K_2(x, x'; t)\,, \tag{10}$$

where

$$K_2(x, x'; t) = \frac{1}{2}\bigg(\chi(0) + \chi(t) + \mathrm{sgn}(x')\int_0^t \mathrm{d}\tau\, \frac{\mathrm{d}\chi(\tau)}{\mathrm{d}\tau}\,\mathrm{erf}(\Phi)\bigg)K_0(x - x', t) \tag{11}$$

and

$$\Phi(x, x'; t, \tau) = \sqrt{\frac{m}{2i\hbar t}}\left(x\sqrt{\frac{\tau}{t - \tau}} + x'\sqrt{\frac{t - \tau}{\tau}}\right)\,. \tag{12}$$

Equations (10–12), while being mathematically equivalent to Eqs. (7–9), enable a straightforward verification of the fact that K satisfies Eqs. (2–5). Indeed, since both K_2 and $\partial_x K_2$ are continuous functions of x, the validity of the discontinuity conditions, Eqs. (4) and (5), follows directly from Eq. (10). The validity of the initial condition, Eq. (3), can be also verified straightforwardly: $K(x,x';0^+) = [\Xi + (1-\Xi)\chi(0)]K_0(x,x';0^+) = \delta(x-x')$. The fact that K satisfies the TDSE is confirmed by a direct substitution of Eqs. (10–12) into Eq. (2). (Here, it is convenient to take into account the identity $\partial_t\Phi + \frac{x-x'}{t}\partial_x\Phi + i\frac{\hbar}{m}\Phi(\partial_x\Phi)^2 = 0$.) Finally, we note that uniqueness of the solution can be established in a standard way [15].

It is important to point out that, due to nonunitarity of quantum evolution in the presence of absorption, the propagator K, in general, does not fulfill the composition property, i.e.,

$$K(x,x';t) \neq \int_{-\infty}^{+\infty} \mathrm{d}\xi\, K(x,\xi;t-\tau)K(\xi,x';\tau)\,. \qquad (13)$$

This can be readily seen by considering the simple case of a time-independent, completely absorbing barrier, for which $\chi = 0$ and $K = \Xi K_0$.

Although not valid generally, the composition property holds in the following important special case. Consider a scenario, in which the absorbing barrier acts only up to some time t_f. In other words, suppose the aperture function χ is such that $\chi(\tau) = 1$ for all $\tau > t_\mathrm{f}$. It can then be shown that K satisfies

$$K(x,x';t) = \int_{-\infty}^{\infty} \mathrm{d}\xi\, K_0(x-\xi,t-\tau)K(\xi,x',\tau) \qquad (14)$$

for $0 < t_\mathrm{f} < \tau < t$. The physical picture offered by Eq. (14) is apparent: Once the absorbing shutter has been switched off, the wave function evolves in accordance with the free-particle propagator.

Equations (7–9) offer the following physical interpretation of the wave function evolution. The full propagator K is a sum of ΞK_0, describing propagation in the case of a completely absorbing barrier ($\chi = 0$), and K_1, representing contribution of a barrier of nonzero transparency. In the transmission region, i.e., for x and x' such that $\Xi(x,x') = 0$, the expression for K_1, Eq. (8), conforms to the Huygens-Fresnel principle [18]: The probability amplitude at the point x and time t, produced by a point source at x' and time 0, can be viewed as that produced by a fictitious source, located at the origin (between x and x'); the strength of the fictitious source is determined by the free-particle wave function at the origin, modulated by the aperture function.

In certain cases, the integral in Eq. (11) can be evaluated explicitly. One important example is that of a "time grating", characterized by a "staircase" aperture function $\chi(\tau) = \chi_0\Theta(t_1-\tau) + \sum_{n=1}^{N-1}\chi_n\Theta(\tau-t_n)\Theta(t_{n+1}-\tau) + \chi_N\Theta(\tau-t_N)$, where $0 \le \chi_j \le 1$, with $0 \le j \le N$, and $0 < t_1 < t_2 < \ldots < t_N < t$. In this case, the integral in Eq. (11) reduces to $\sum_{n=1}^{N}(\chi_{n+1}-\chi_n)\mathrm{erf}[\Phi(x,x';t;t_n)]$, rendering a closed form expression for the propagator. In particular, $\chi(t) = \Theta(t-t_1)$ leads to a propagator coincident with that in the original Moshinsky's shutter problem [18].

A diffracted wave function, $\Psi(x,t)$, resulting from an arbitrary initial state, $\Psi_0(x)$, can now be obtained by numerically evaluating the integral in Eq. (1). As an illustration, we consider diffraction of an initially localized Gaussian wave packet. Adopting atomic units, $m = \hbar = 1$, we consider a coherent state $\psi_{q,p}(x) = (\pi)^{-1/4}\exp[-\frac{1}{2}(x-q)^2 + ip(x-q)]$, with the average position q and momentum p, and set the initial state to be $\Psi_0(x) = \psi_{-10,\,5}(x)$. Figure 2 shows the wave function $\Psi(x,t)$ at time $t = 3$ diffracted at two different time gratings $\chi(\tau)$, shown in the insets of Figs. 2a and 2c. The elementary, one-period cell of the first grating, Fig. 2a, is given by $0\times\Theta(\tau)\Theta(\Delta t-\tau) + 1\times\Theta(\tau-\Delta t)\Theta(2\Delta t-\tau)$, and that of the second grating, Fig. 2c, by $0\times\Theta(\tau)\Theta(\Delta t-\tau) + 0.5\times\Theta(\tau-\Delta t)\Theta(2\Delta t-\tau) + 1\times\Theta(\tau-2\Delta t)\Theta(3\Delta t-\tau)$, with $\Delta t = 0.056$. (The value $\chi = 0.5$ means that the shutter allows only a half of the probability amplitude through, while absorbing the other half.) The probability densities $|\Psi(x,t)|^2$ for the two gratings are shown in the main panels of Figs. 2a and 2c, and the corresponding Husimi distributions, $H(q,p) = \left|\int_{-\infty}^{+\infty}\mathrm{d}x\,\psi^*_{q,p}(x)\Psi(x,t)\right|^2$, with the asterisk denoting complex conjugation, are presented in Figs. 2b and 2d, respectively. (Phase-space representations, akin to $H(q,p)$, have been previously used for establishing classical-quantum analogies in the dynamics of diffracted particles [19].) The central bright peaks in Figs. 2b and 2d are localized around the point $(q,p) = (5,5)$, which is the average phase-space location of the particle in the absence of a shutter. Additionally, in the case of the first grating, three separated diffraction peaks – one in the reflection region, $q < 0$, and two in the transmission region, $q > 0$, – are clearly visible in Fig. 2b. On the contrary, in the case of the second grating, Fig. 2d, diffraction peaks overlap substantially, forming a distinct pattern of probability naughts, i.e., points in phase space "avoided" by the diffracted particle. We point out that, in general, the diffraction pattern sensitively depends on the initial wave packet and aperture function, making diffraction on time gratings well suited for spectroscopic analysis of quantum states.

So far, we have shown that Eqs. (7–9), or equivalently Eqs. (10–12), give an exact solution to a quantum dynamical problem, defined by Eqs. (2–5). A natural question is however in order: Does this dynamical system accurately model physical reality? In what follows, we argue that the proposed system should indeed provide a good description of the motion of a quantum particle in the presence of a purely absorbing (but not reflecting, in the

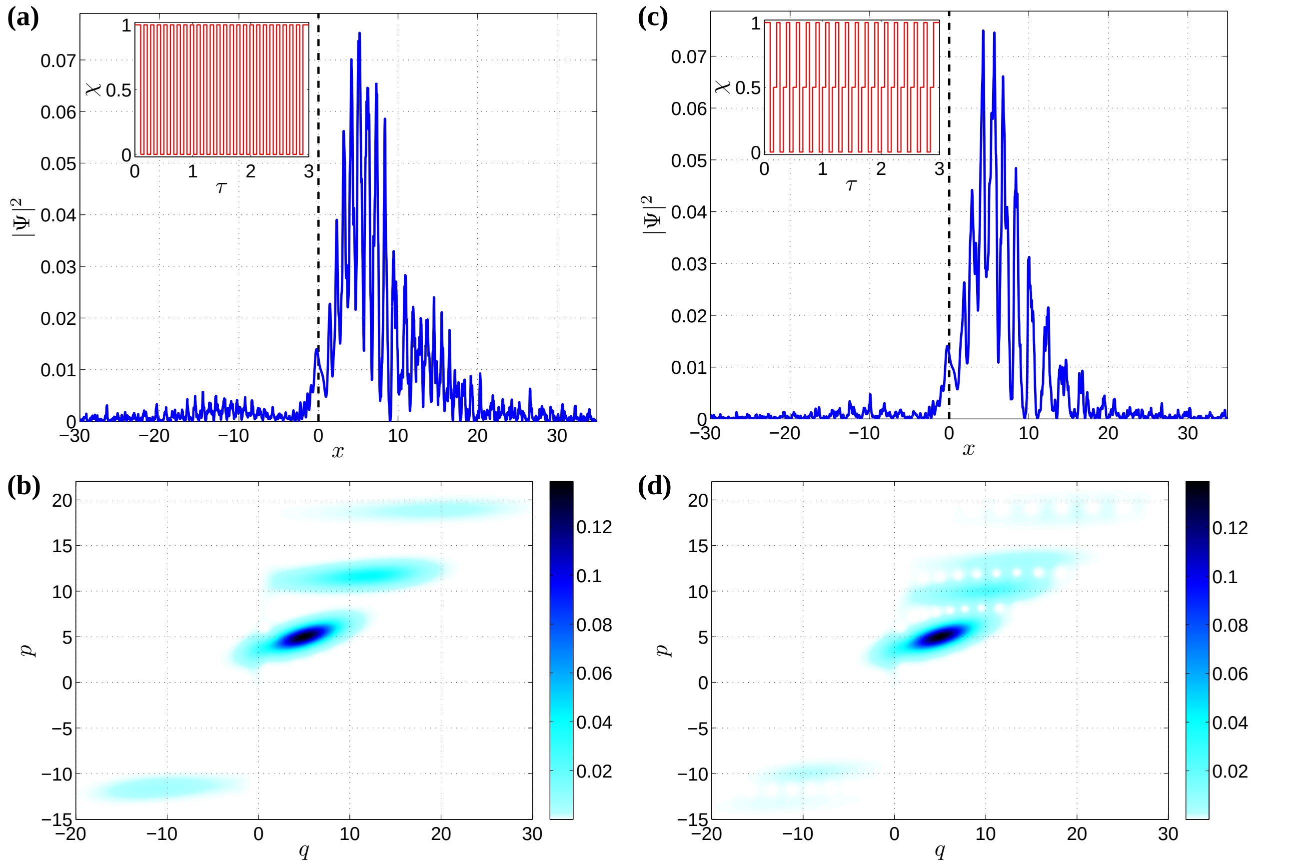

FIG. 2: Diffraction in time of an initially Gaussian wave packet. Figures (a) and (b) show, respectively, the probability density and Husimi representation of the diffracted wave packet for the aperture function given in the inset of (a). Similarly, figures (c) and (d) correspond to the aperture function given in the inset of (c). All quantities are given in atomic units, $m = \hbar = 1$.

classical sense) barrier. The key building block of our model is a time-dependent extension of the Kottler's discontinuity conditions, Eqs. (4) and (5). The latter, in the case of stationary waves governed by the Poisson's equation, are mathematically equivalent to Kirchhoff's description of diffraction. Predictions of the Kirchhoff's theory, in turn, are generally found in good agreement with experimental data in the transmission region, while somewhat lacking accuracy in the reflection region [20]. Therefore, at the very least, it is reasonable to expect the propagator $K(x, x'; t)$ to correctly describe quantum wave dynamics in the transmission region. Moreover, if the absorbing shutter is in effect only until some final time t_f, so that $\chi(t) = 1$ for all $t > t_\mathrm{f}$, then $K(x, x'; t)$, being an analytic function of x at any time $t > t_\mathrm{f}$, must correctly describe the dynamics of the diffracted particle in both the transmission and the reflection regions.

Nevertheless, in the absence of a compelling local theory of absorption, the ultimate answer to the question of how accurately the proposed model describes physical reality can only be given by an experimental investigation. To this end, atom-optics systems appear to be particularly suitable. Remarkably, recent progress in control and manipulation of ultra-cold atoms has made it possible to perform diffraction and interference experiments with a single, isolated atom, corresponding to a quantum wave packet highly localized in space [21]. At the same time, strong ionizing radiation has been used to realize an optical diffraction grating, similar in effect to an absorbing nanostructure (mechanical) grating [22]. Utilizing these technologies, one might envision a single-atom DIT experiment, in which quasi-one-dimensional motion of an atom is "intercepted" by a time-dependent absorbing shutter produced by a transversely-oriented, pulsing sheet of ionizing radiation.

In conclusion, we have addressed a self-consistent mathematical model of diffraction in time and found its exact analytical solution in form of a time-dependent propagator. The latter enables a quantitative description of diffraction of an arbitrary initial quantum state at an absorbing shutter governed by an arbitrary aperture function. We believe that our model will prove useful in the areas of coherent quantum control, quantum metrology, in designing new diffraction and interference experiments with atoms and molecules, and, more generally, in exploring foundations of quantum physics.

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